論文の内容の要旨

Effect of the electronic entropy on structural change and ablation of metals by an ultrashort laser pulse

(超短パルスレーザが照射された金属の構造変化とアブレーションに対する電子エントロピーの効果)

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Irradiation of a solid surface with an ultrashort laser pulse creates a highly excited state, where a high-energy electron system (~ eV) coexists with a low-energy lattice system. In this nonequilibrium state, some specific phenomena have been reported such as the emission of excessively high-energy atoms/ions and less than nm order ablation. These phenomena are called a non-thermal ablation and have been particularly focused on from not only fundamental physics but also applied physics since the understanding of it directly leads to the development of the higher precision processing technique. Despite intensive investigation inspired by its interest and importance, its physical mechanism is an open question, and there is discrepancy between experiments and previous theoretical simulations.

Purposes of our study are following two. The first one is bridging this discrepancy by elucidating the physical mechanism of the non-thermal ablation of metals. The other is extending calculation models and developing codes to simulate the irradiated metal with an ultrashort pulse laser.

Throughout our study, we use the well-known two-temperature model (TTM) to describe irradiated metals with an ultrashort laser pulse. Our finite-temperature density functional theory (FTDFT) calculations show that the electronic entropy effect leads to the instability of condensed copper (Cu) at high electronic temperature. Based on the result, we propose the electronic entropy-driven (EED) mechanism to describe the non-thermal ablation of metals. Subsequently, to investigate the physical mechanism of the non-thermal ablation and the validity of the EED

mechanism, we extend simulation methods and develop calculation codes of the continuum model (CM) simulation and the TTM molecular dynamics (TTM-MD) simulation. Our simulations reproduce experimental results, such as the fluence dependence of the ablation depth and the emission of the high-energy atoms. These results strongly support that the origin of the driving force of the high-energy atom emission is attributed to the electronic entropy effect and the validity of the EED mechanism. In addition, we construct a simple calculation model for estimating the ablation threshold fluence based on our CM and TTM-MD simulation results to find reasonable agreement for several materials (Cr, W, Mo, Ni, Pt, Al, Ag, Cu, and Au).

We are sure that our findings include fundamentally important knowledge not only for the ablation issue but also for the warm dense matter physics and the ultrafast physics, and provide new and essential insight into these interdisciplinary fields. Moreover, our extended calculation models and developed codes will continue to promote the further understanding these fields.